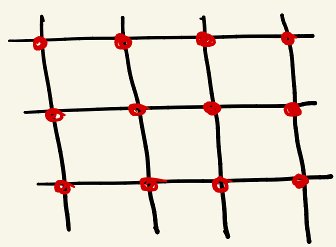
A general relation between ground state degeneracy and filling

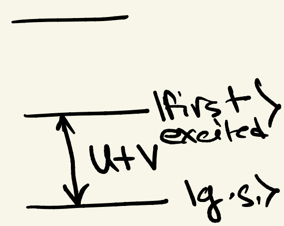
(Oshikawa's flux threading argument, cond-mat/9911137)

Motivation: Consider Bose-Hubbard model on a square lattice with onsite as well as nearest-neighbor interaction:

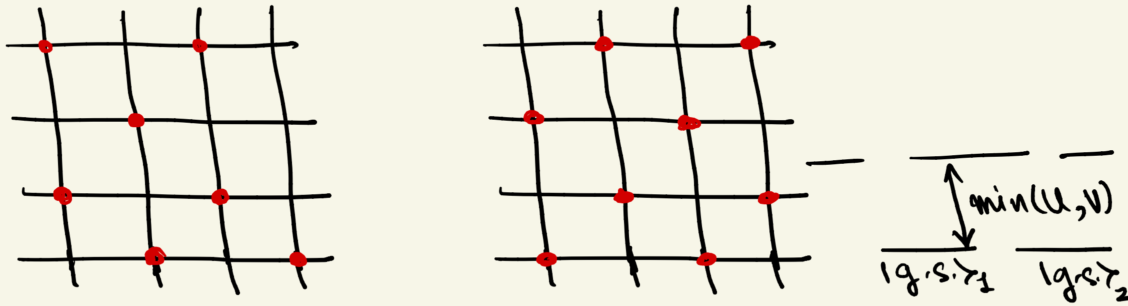
$$H = -t\sum_{\langle ij\rangle}(b^\dagger_i b_j + h.c.) + U\sum_i n_i^2 + V\sum_i n_i n_{i+1}$$ with

$\frac{U}{t}, \frac{V}{t} \to \infty$. If the filling $\left(= \frac{\#\text{ of particles}}{\#\text{ of sites}}\right)$ is one, then one can clearly write down a unique ground state at large interaction strength U:



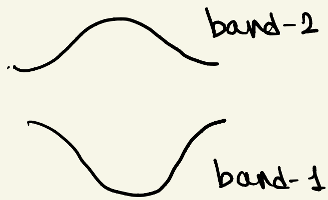


On the other hand when the filling is $\frac{1}{2}$, then there are <u>two</u> ground states (recall we are in the limit $\frac{U}{t}, \frac{V}{t} \to \infty$) :



i.e. all particles live either on the A sublattice or the B sublattice. It's natural to wonder if the increase in the number of ground states (from one to two) as the filling changes from unity to $\frac{1}{2}$ is a special feature of this specific Hamiltonian or is it somehow more general?

As another example, consider non-interacting electrons in a periodic potential so that they form bands:



To obtain a band insulator, one again needs an integer filling so that the lower band (= band-1) is fully filled. In contrast, when the filling is $\frac{1}{2}$, one would obtain a metal. We again see that to obtain a unique ground state separated from the rest of the spectrum with a non-zero gap in the thermodynamic limit, one needs an integer filling.

Remarkably, one can show (Oshikawa 1999) that at filling $\frac{p}{q}$ where p and q are co-primes, there must exist q low-lying states (i.e. states whose energy difference with each other vanishes in the thermodynamic limit). The only assumption is that the system has translation × particle no. conservation sym.

Oshikawa's proof of the above statement:

Let's impose periodic boundary conditions on the system along the x-direction (other directions can have periodic or open boundaries, it doesn't matter). The Hamiltonian preserves Translation $\times$ particle no. conservation sym, and no other assumptions are made.

The main idea is to couple the system to a background guage field that has a non zero flux $\oint \vec{A} \cdot \vec{dl}$ where the loop in the integral $\oint$ is along the x-direction (the same direction along which PBC are imposed).

For example, if in the absence of the background flux, Hamiltonian is

$$H = -t \sum_{\langle ij \rangle} (c^+_i c_j + h.c.) + H_{int}(\{c^+_i c_i\})$$

where H_{int} is any term that depends on the particle density (e.g. $V\sum_i n_i n_{i+1}$), then in the presence of flux ϕ,

$$H(\phi) = -t \sum_{\langle ij \rangle} (c^+_i c_j e^{i A_{ij}} + h.c.) + H_{int}$$

where $A_{ij} = \frac{\phi}{L_x}$ for ij nearest neighbors along the x-direction, and $A_{ij} = 0$ otherwise. This ensures that $\oint \vec{A} \cdot d\vec{l} = \phi$ for any loop along the x-direction.

In the following, for concreteness, we will take the Hamiltonian of the form written above i.e. $H = -t \sum_{\langle ij \rangle} (c^+_i c_j + h.c.) + H_{int}(\{c^+c\})$

Let's start from the Hamiltonian at zero flux $H(\phi=0)$ whose ground state is denoted as $|\psi(\phi=0)\rangle$. One <u>adiabatically</u> increases the flux from 0 to 2π.

Adiabatic theorem implies that the state at flux ϕ will be the ground state of $H(\phi)$ i.e. $H(\phi)|\psi(\phi)\rangle = \epsilon|\psi(\phi)\rangle$.

Interestingly, the ground state energy of $H(\phi=2\pi)$ is identical to $H(\phi=0)$. One way to see this is that one can write down an explicit unitary operator U such that $U^{\dagger} H(\phi=2\pi) U = H(\phi=0)$, which implies that the spectrum of $H(\phi=2\pi)$ = spectrum of $H(\phi=0)$. We will construct U below. An alternative way to arrive at the same conclusion is to note that the interaction part of H is independent of the flux, while the hopping part is

$$H_0 = -t \sum_k \left[\cos\left(k_x + \frac{\phi}{L_x}\right) + \cos(k_y)\right] c^+(k_x, k_y)\, c(k_x, k_y).$$

The allowed values of $k_x = \frac{2\pi n}{L_x}$ and therefore, when $\phi = 2\pi$, one simply shifts the energy levels by one lattice spacing in the momentum space, and the spectrum is unchanged.

Therefore,

$$H(\phi=0)\,|\psi(\phi=0)\rangle = E_0\,|\psi(\phi=0)\rangle$$

and

$$H(\phi=2\pi)\,|\psi(\phi=2\pi)\rangle = E_0\,|\psi(\phi=2\pi)\rangle$$

where we have denoted $E(\phi=0) = E(\phi=2\pi)$ as E_0. Note, crucially, that $|\psi(\phi=0)\rangle \neq |\psi(\phi=2\pi)\rangle$.

Another important constraint is that since $[H(\phi), \hat{T}_x] = 0 \;\forall\, \phi$ where $\hat{T}_x$ is the unitary operator that generates translation along the x-direction, the eigenvalue of $\hat{T}$ is unchanged during the flux threading operation.

One can see this explicitly :

$$\hat{T}\,|\varphi(\phi)\rangle = \hat{T}\, e^{-iH(\phi)dt}\, e^{-iH(\phi-d\phi)dt} \cdots e^{-iH(\phi=0)\,dt}\,|\varphi(\phi=0)\rangle$$

$$= e^{-iH(\phi)dt}\, e^{-iH(\phi-d\phi)\,dt} \cdots e^{-iH(\phi=0)dt}\,\hat{T}\,|\varphi(\phi=0)\rangle$$

If $\hat{T}\,|\varphi(\phi=0)\rangle = e^{iP_{0x}}\,|\varphi(\phi=0)\rangle$

$\Rightarrow \hat{T}\,|\varphi(\phi)\rangle = e^{iP_{0x}}\,|\varphi(\phi)\rangle$

where P_{0x} is just a number.

Now we will show that when the filling is $\frac{p}{q}$ with p, q co-primes, then one can find q states that have energy E_0 and which all differ in momentum. Since momentum is a good quantum number, this implies that the ground state degeneracy is atleast q. To show this, we first find the promised unitary $\mathcal{U}$ that relates $H(\phi=0)$ and $H(\phi=2\pi)$. Since $H(\phi=2\pi)$ is just $H(\phi=0)$ with shift of $\frac{2\pi}{L_x}$ in the momentum space, one would guess that the unitary looks like

$$\mathcal{U} = e^{\frac{2\pi i}{L_x} \sum_{x,y} x \, \hat{n}(x,y)}$$

where $\hat{n}(x,y) = c^{\dagger}(x,y)\, c(x,y)$ is the density operator on site (x,y). This guess is indeed correct. Consider, for example the hopping term between (x,y) and $(x+1,y)$ in $H(\phi=2\pi)$:

$$h = c^\dagger(x,y)\, c(x+1,y)\, e^{i\frac{2\pi}{L_x}}$$

$$\Rightarrow U h U^\dagger = U c^\dagger(x,y) U^\dagger \; U c(x+1,y) U^\dagger \, e^{\frac{2\pi i}{L}}$$

Now, $U c^\dagger(x,y) U^\dagger = e^{\frac{2\pi i x}{L_x}} c^\dagger(x,y)$

while $U c(x+1,y) U^\dagger = e^{-\frac{2\pi i(x+1)}{L_x}} c(x+1,y)$

following the calculation identical to that in pset-1.

$$\Rightarrow U h U^\dagger = c^\dagger(x,y)\, c(x+1,y)$$

$$\Rightarrow U H(\phi=2\pi) U^\dagger = H(\phi=0).$$

Now let's calculate the energy and momentum of the state $\mathcal{U}|\psi(\phi=2\pi)\rangle$

Energy: $H(\phi=0)\,\mathcal{U}\,|\psi(\phi=2\pi)\rangle$

$$= \mathcal{U}\,\underbrace{\mathcal{U}^{\dagger}\,H(\phi=0)\,\mathcal{U}}\,|\psi(\phi=2\pi)\rangle$$

$$= \mathcal{U}\;H(\phi=2\pi)\,|\psi(\phi=2\pi)\rangle$$

$$= E_0\;\mathcal{U}|\psi(\phi=2\pi)\rangle.$$

$\Rightarrow$ $\mathcal{U}|\psi(\phi=2\pi)\rangle$ has the same energy as the ground state.

Momentum: $\hat{T}\;\mathcal{U}\,|\psi(\phi=2\pi)\rangle$

$$= \hat{T}\,\mathcal{U}\,\hat{T}^{\dagger}\,T\,|\psi(\phi=2\pi)\rangle$$

$\hat{T}\,\mathcal{U}\,\hat{T}^{\dagger}$ is just translated version of $\mathcal{U}$.

Since $\mathcal{U} = e^{\frac{2\pi i}{L_x}\sum_{x,y} x\, c^{\dagger}(x,y)\, c(x,y)}$

$$\hat{T}\,\mathcal{U}\,\hat{T}^{\dagger} = e^{\frac{2\pi i}{L_x}\sum_{x,y} x\, c^{\dagger}(x+1,y)\, c(x+1,y)}$$

$$= e^{2\pi i/L_x \sum_{x,y}\left[(x+1)\, c^{\dagger}(x+1,y)\, c(x+1,y) - c^{\dagger}(x+1,y) c(x+1,y)\right.}$$

$$= U\, e^{-\frac{2\pi i}{L_x} \sum_{x,y} c^{\dagger}(x+1,y)\, c(x+1,y)}$$

$$= U\, e^{-\frac{2\pi i N}{L_x}} = U\, e^{-2\pi i \nu L_y}$$

where $\nu = \frac{N}{L_x L_y} = \frac{p}{q}$ is the filling.

$$\Rightarrow \hat{T}\, U\, |\psi(\phi = 2\pi)\rangle = e^{-2\pi i \nu L_y + i P_{0x}}\, U\, |\psi(\phi = 2\pi)\rangle$$

$\Rightarrow$ The state $U|\psi(\phi=2\pi)\rangle$ carries a momentum of $P_{0x} - \frac{2\pi p}{q} L_y$.

Let's <u>choose</u> L_y that is not a multiple of q (i.e. q and L_y are co-prime).

$$\Rightarrow P_{0x} - \frac{2\pi p}{q} L_y \neq P_{0x} + 2\pi \times \text{integer}$$

(recall that the lattice momentum is defined only upto $2\pi \times$ integers).

$\Rightarrow$ The state $U|\psi(\phi = 2\pi)\rangle$ <u>must</u> be orthogonal to $|\psi(\phi=0)\rangle$ while having the same energy.

Similarly, consider the state $\mathcal{U}^2 |\psi(\phi=2\pi)\rangle$. Following identical argument, it will have energy E_0 and momentum $P_{0x} - 2 \times \frac{2\pi p}{q} L_y$.

Repeating the process $q-1$ times generates $q-1$ states with energy E_0 that all have different momenta from $|\psi(\phi=0)\rangle$.

$\Rightarrow$ One obtains q states that have energy E_0 and distinct momenta

$$|\psi(\phi=0)\rangle, \ \mathcal{U}|\psi(\phi=2\pi)\rangle, \ \mathcal{U}^2|\psi(\phi=2\pi)\rangle, \ \ldots \ \mathcal{U}^{q-1}|\psi(\phi=2\pi)\rangle.$$

This concludes the proof.